

SUPPLEMENTARY MATERIAL

Four new compounds from *Neoboletus magnificus*

Zhi Yang^a, Ying-tong Di^b, Yu Zhang^b, Xu-Jia Hu^a *

^aFaculty of Life Science and Technology, Kunming University of Science and Technology, Kunming, 650500, China; ^bState Key Laboratory of Phytochemistry and Plant Resources in West China, Kunming Institute of Botany, Chinese Academy of Science, Kunming, 650204, China

ABSTRACT

Four new compounds, compounds **1**, **2**, **4**, **6**, along with two compounds **3**, **5**, were isolated from the methanol extract of the fruiting body of *Neoboletus magnificus*. The structures of compounds were elucidated by HRMS and NMR spectroscopic methods. The *in vitro* anti-inflammatory activity of the isolated compounds was evaluated.

Key words: *Neoboletus magnificus*, Boletaceae, sphingolipid, pyrrole alkaloid

Contents

Figure S1. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **1**

Figure S2. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **2**

Figure S3. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **3**

Figure S4. Key ^1H - ^1H COSY and HMBC correlations for compounds **4-5**

Figure S5. Key ^1H - ^1H COSY and HMBC correlations for **6**

Figure S6- S7. 1D NMR spectra of compound **1** in CD_3OD .

Figure S8- S10. 2D NMR spectra of compound **1** in CD_3OD .

Figure S11- S12. 1D NMR spectra of compound **2** in $\text{DMSO}-d_6$.

Figure S13- S15. 2D NMR spectra of compound **2** in DMSO- d_6 .

Figure S16- S17. 1D NMR spectra of compound **3** in DMSO- d_6 .

Figure S18- S20. 2D NMR spectra of compound **3** in DMSO- d_6 .

Figure S21- S22. 1D NMR spectra of compound **4** in DMSO- d_6 .

Figure S23- S25. 2D NMR spectra of compound **4** in DMSO- d_6 .

Figure S26- S27. 1D NMR spectra of compound **5** in Acetone.

Figure S28- S30. 2D NMR spectra of compound **5** in Acetone.

Figure S31- S32. 1D NMR spectra of compound **6** in DMSO- d_6 .

Figure S33- S35. 2D NMR spectra of compound **6** in DMSO- d_6 .

Table S1. ^1H and ^{13}C NMR Data (δ) of Compound **1** (δ in ppm and J in 800 Hz) in CD_3OD .

Table S2. ^1H and ^{13}C NMR Data (δ) of Compound **2** (δ in ppm and J in 600 Hz) in DMSO- d_6 .

Table S3. ^1H and ^{13}C NMR Data (δ) of Compound **3** (δ in ppm and J in 600 Hz) in DMSO- d_6 .

Table S4. ^1H and ^{13}C NMR Data (δ) of Compound **4** (δ in ppm and J in 500 Hz) in DMSO- d_6 .

Table S5. ^1H and ^{13}C NMR Data (δ) of Compound **5** (δ in ppm and J in 600 Hz) in Acetone.

Table S6. ^1H and ^{13}C NMR Data (δ) of Compound **6** (δ in ppm and J in 600 Hz) in DMSO- d_6 .

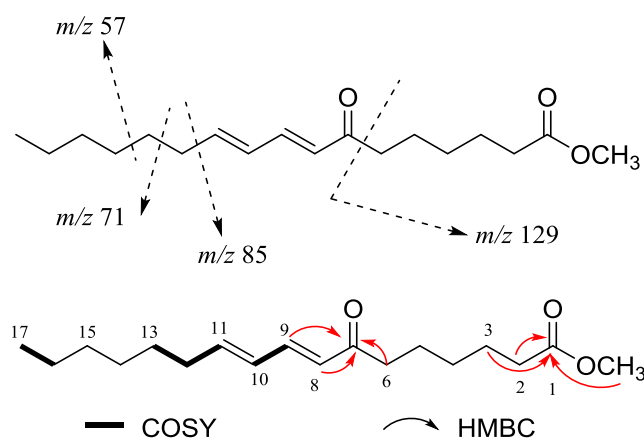


Figure S1. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **1**

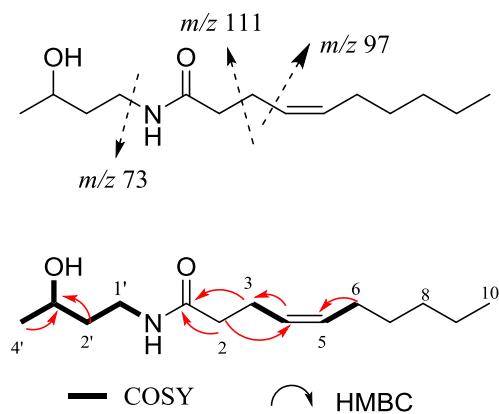


Figure S2. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **2**

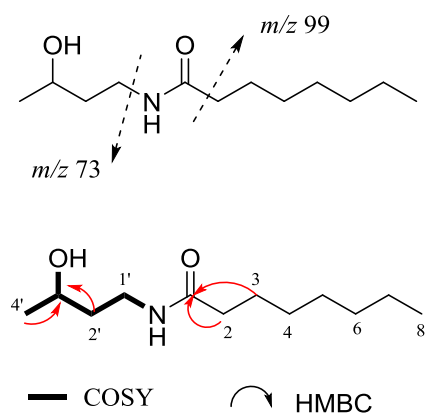


Figure S3. EIMS fragmentation, key ^1H - ^1H COSY and HMBC correlations for **3**

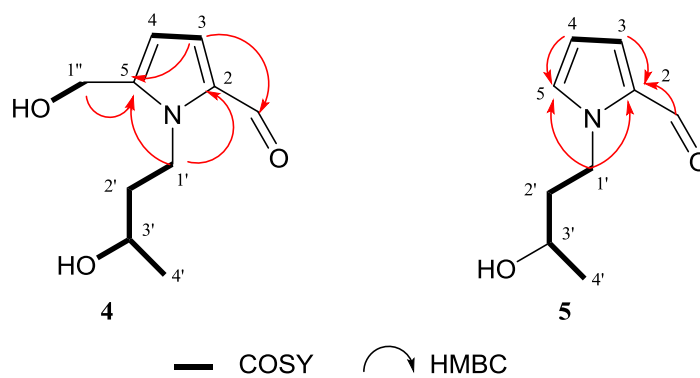


Figure S4. Key ^1H - ^1H COSY and HMBC correlations for compounds 4-5

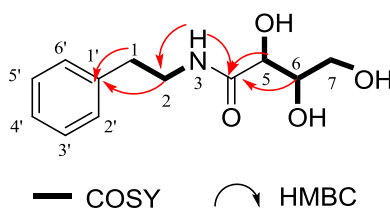


Figure S5. Key ^1H - ^1H COSY and HMBC correlations for 6

Figure S6. ^1H NMR spectrum of compound 1 (CD_3OD) .

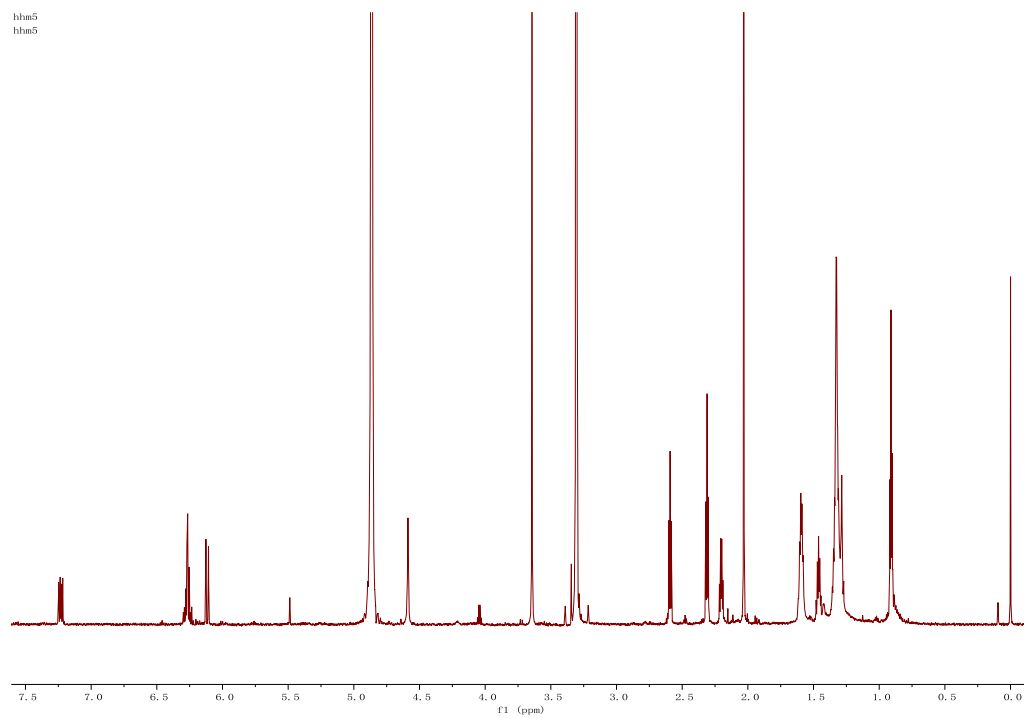


Figure S7. ^{13}C NMR and DEPT spectrum of compound **1** (CD_3OD) .

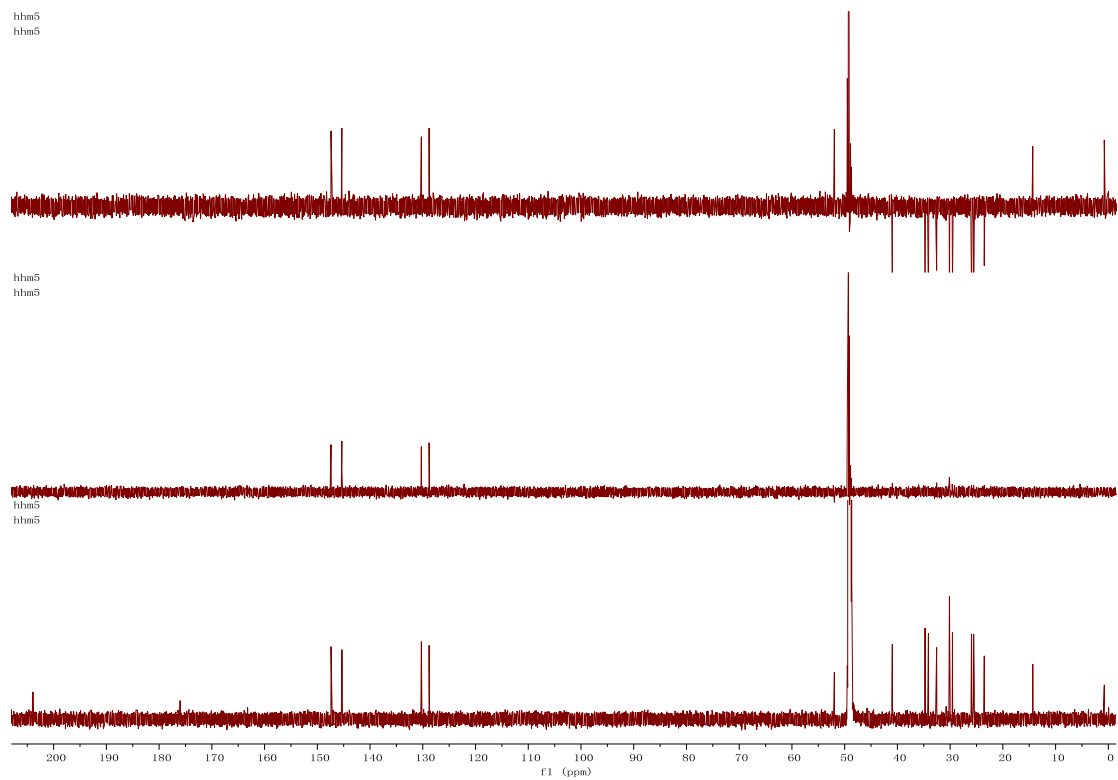


Figure S8. HSQC spectrum of compound **1** .

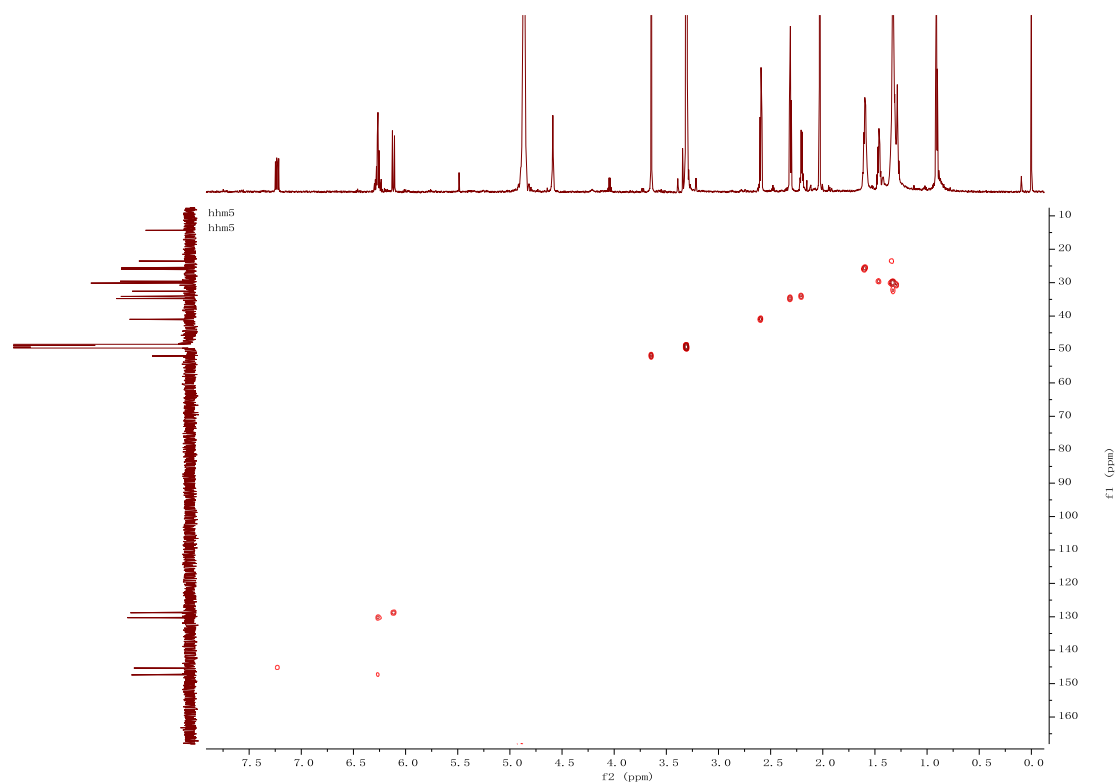


Figure S9. HMBC spectrum of compound **1** .

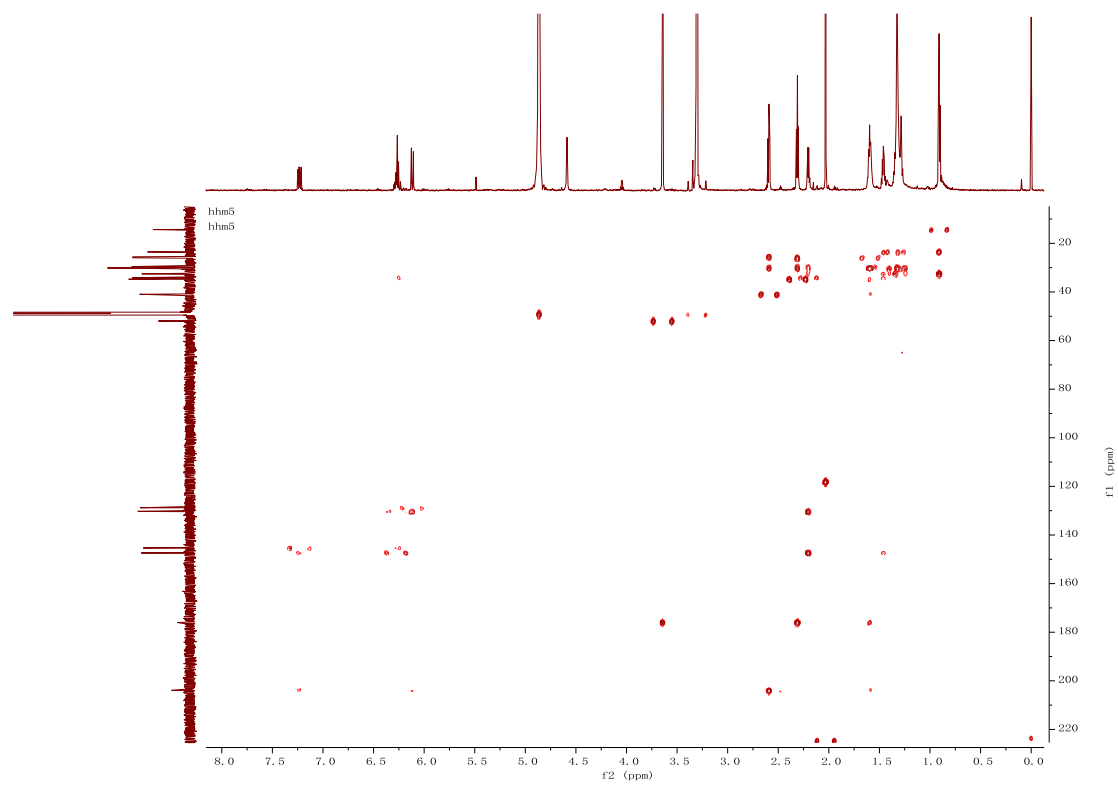


Figure S10. ^1H - ^1H COSY spectrum of compound **1** .

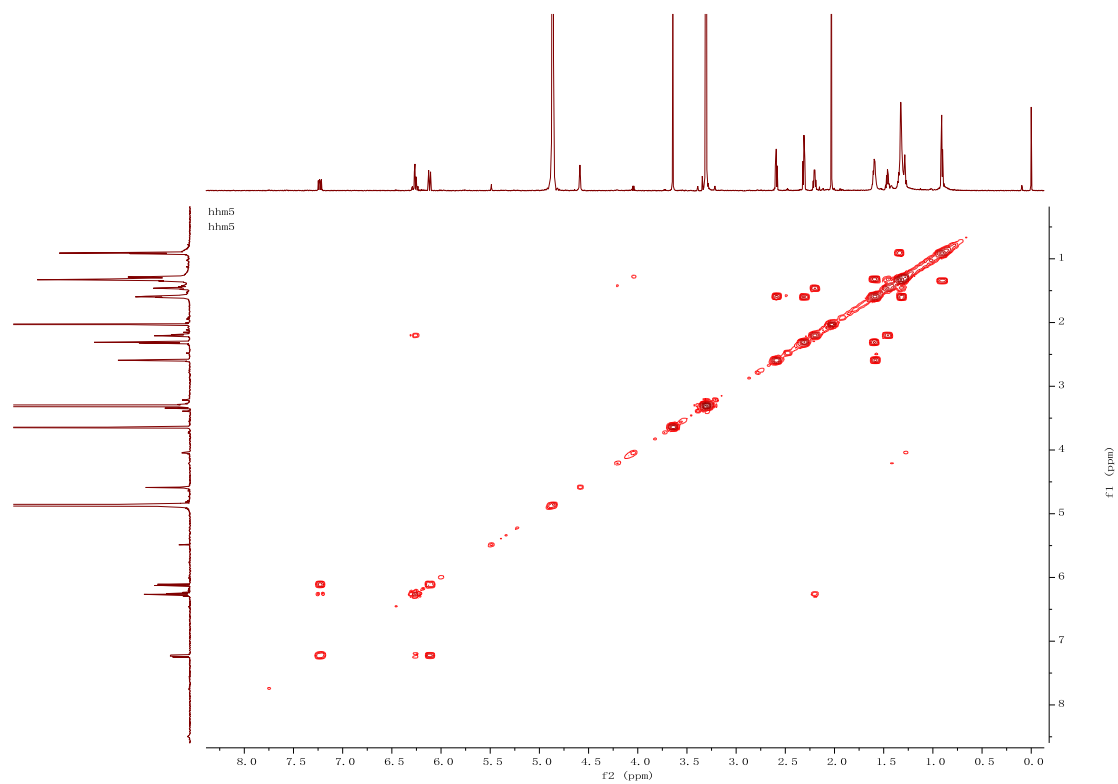


Figure S11. ^1H NMR spectrum of compound **2** ($\text{DMSO}-d_6$) .

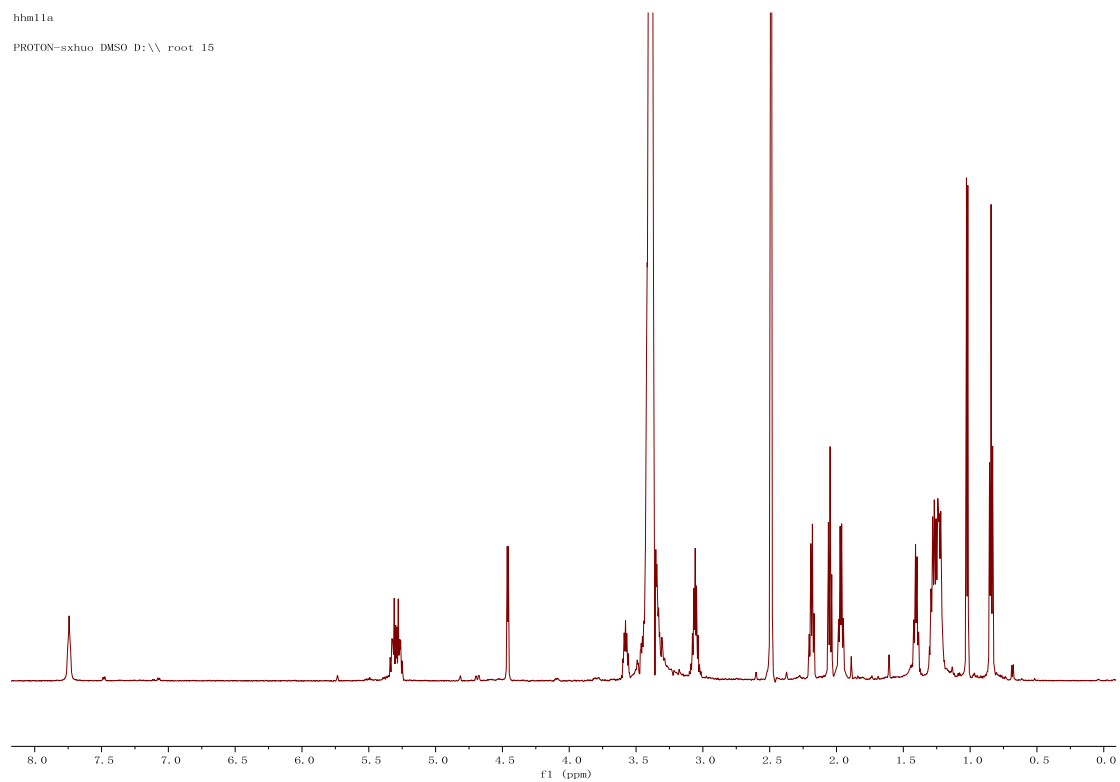


Figure S12. ^{13}C NMR and DEPT spectrum of compound 2 ($\text{DMSO}-d_6$) .

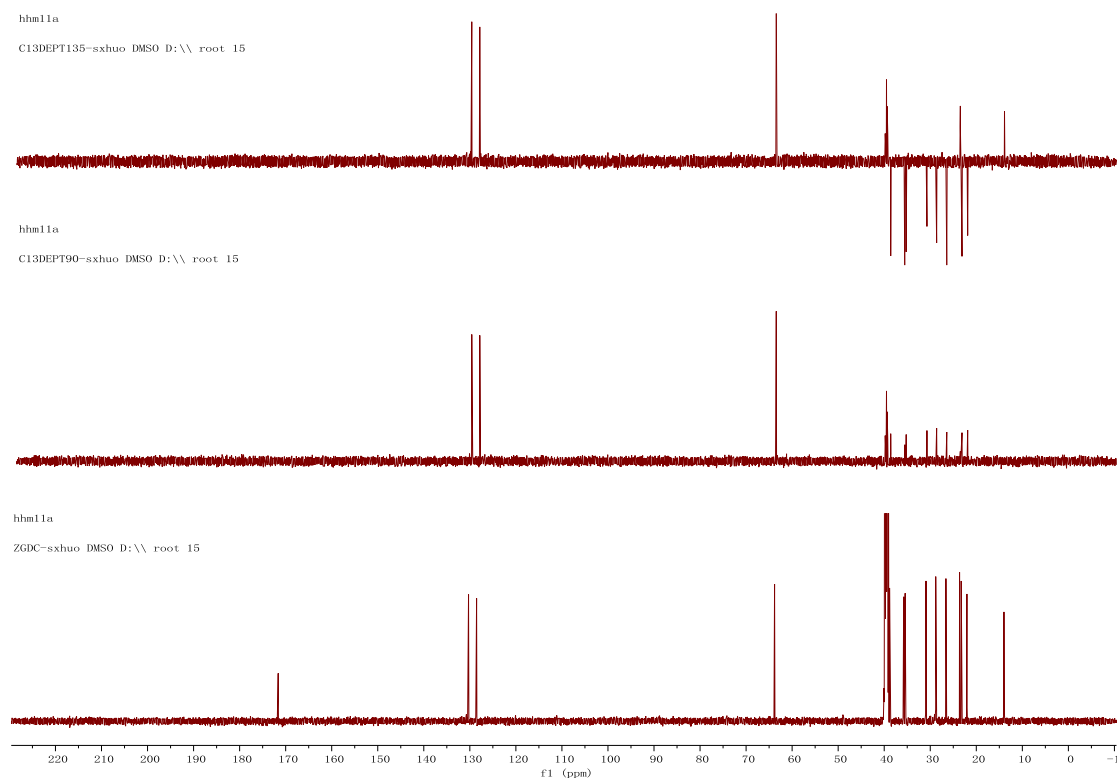


Figure S13. HSQC spectrum of compound 2 .

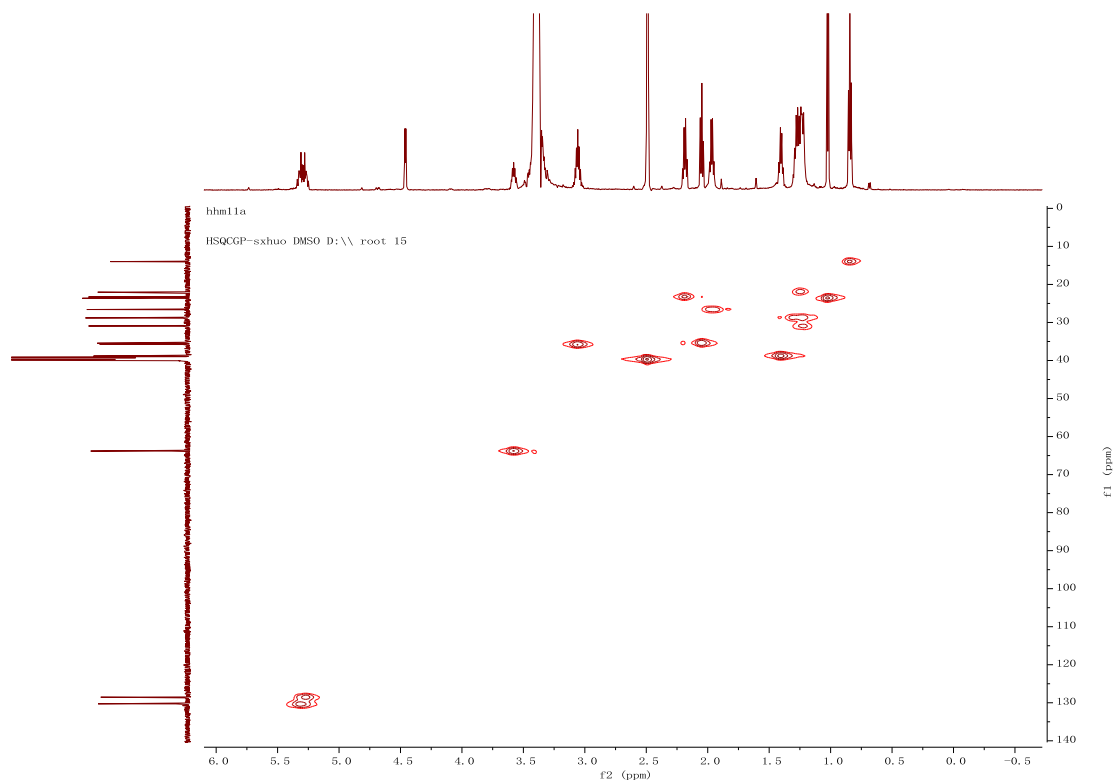


Figure S14. HMBC spectrum of compound **2** .

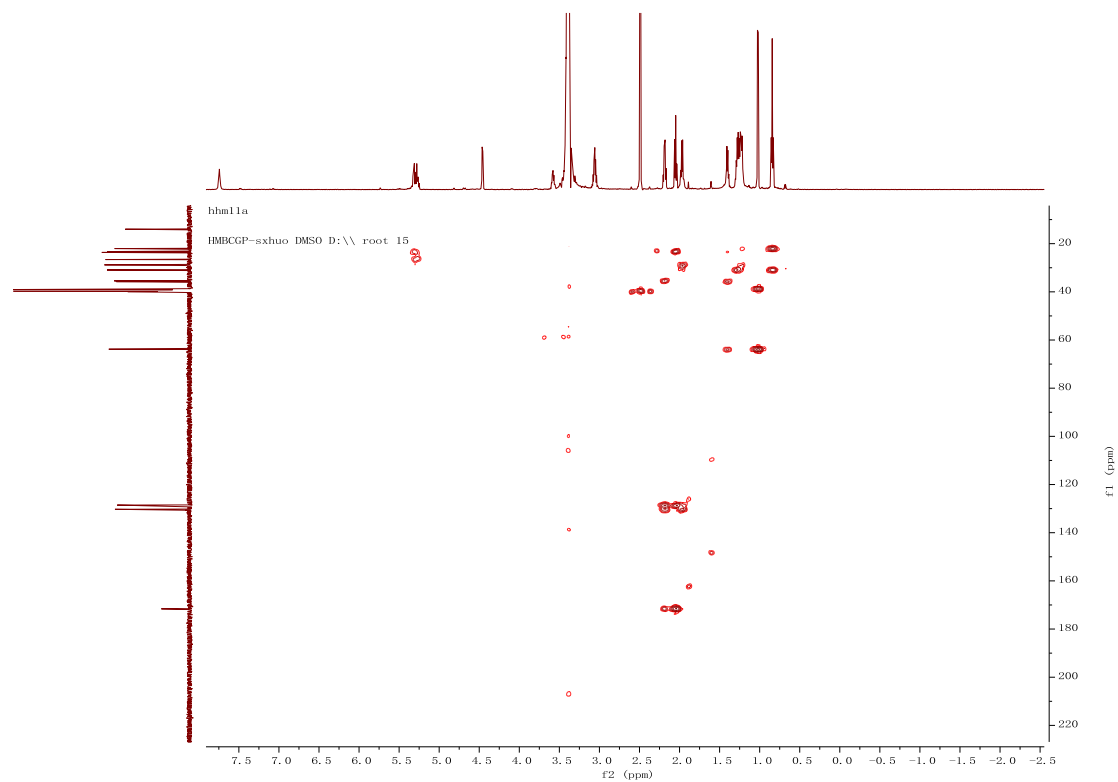


Figure S15. ^1H - ^1H COSY spectrum of compound **2** .

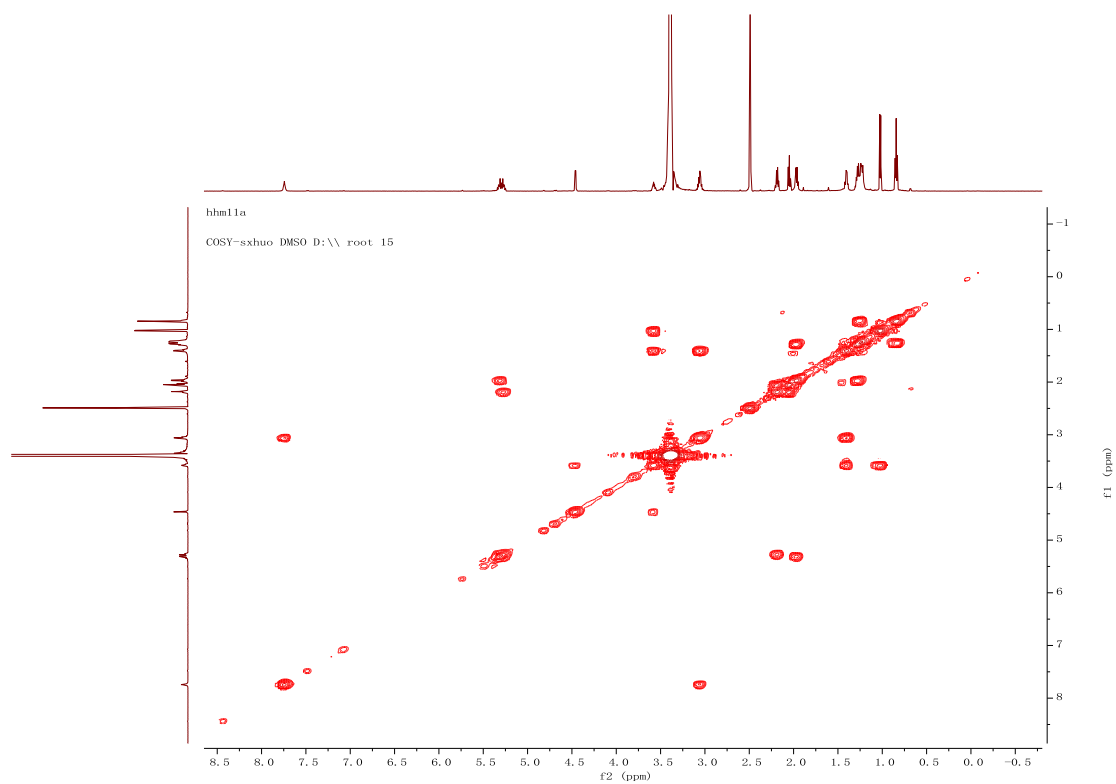


Figure S16. ^1H NMR spectrum of compound 3 ($\text{DMSO}-d_6$).

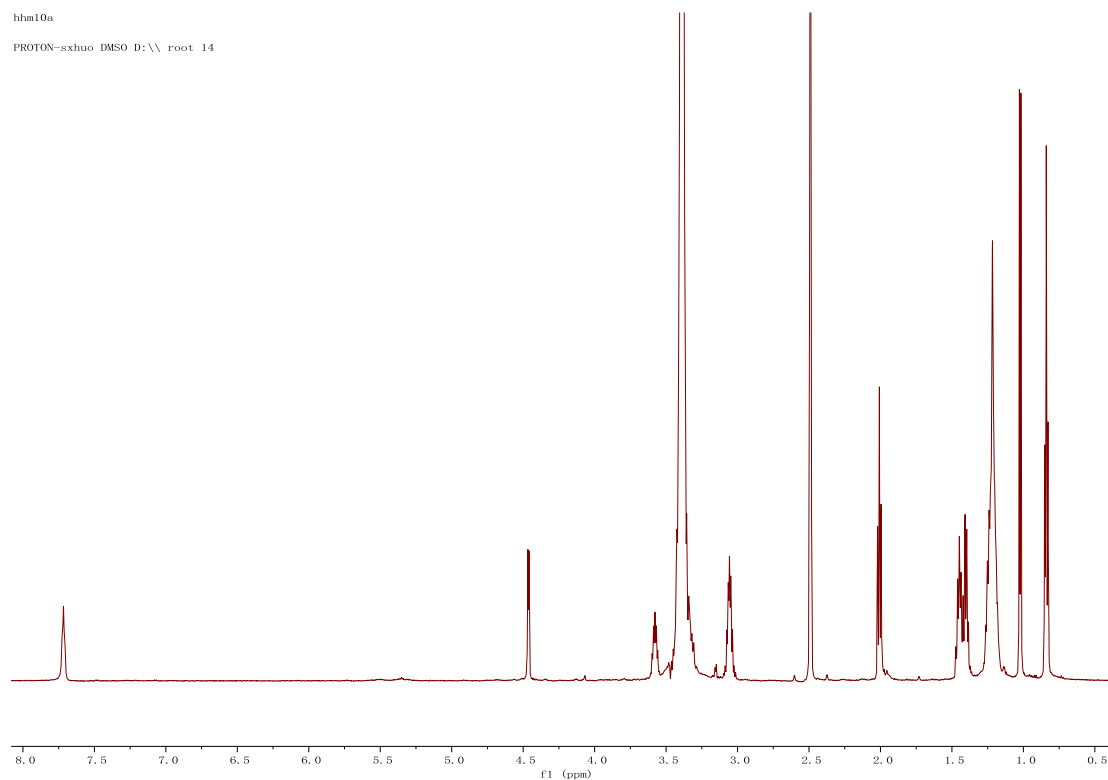


Figure S17. ^{13}C NMR and DEPT spectrum of compound **3** ($\text{DMSO-}d_6$).

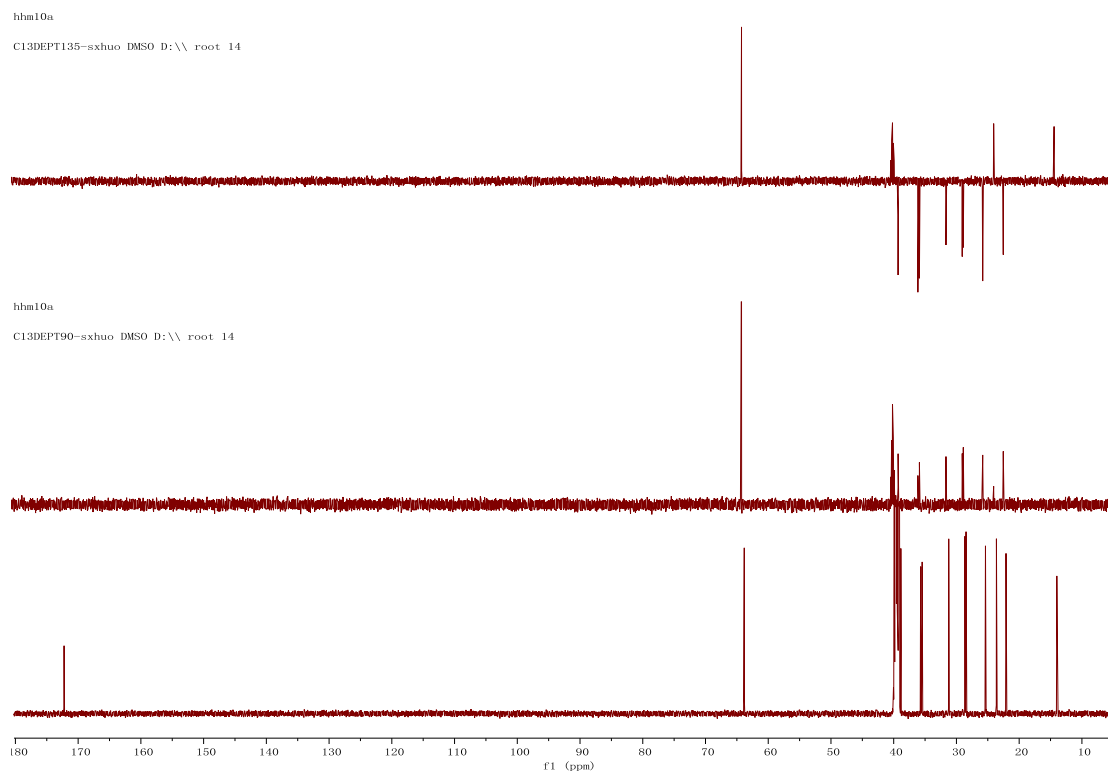


Figure S18. HSQC spectrum of compound **3** .

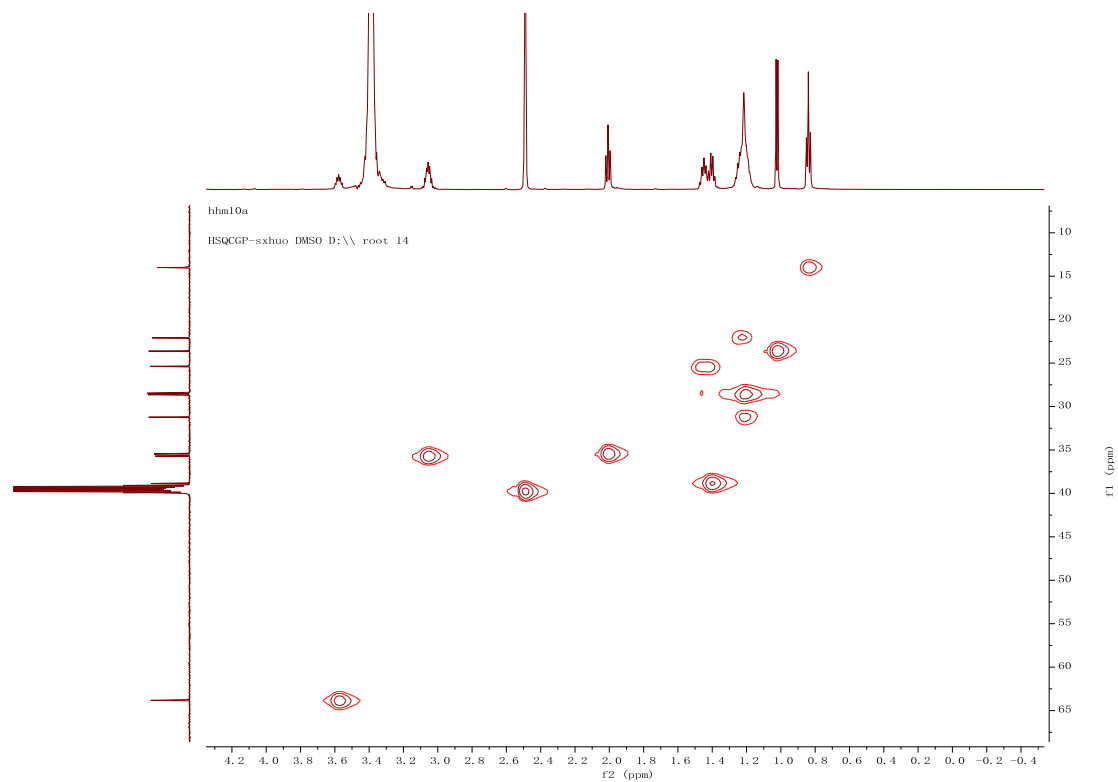


Figure S19. HMBC spectrum of compound **3** .

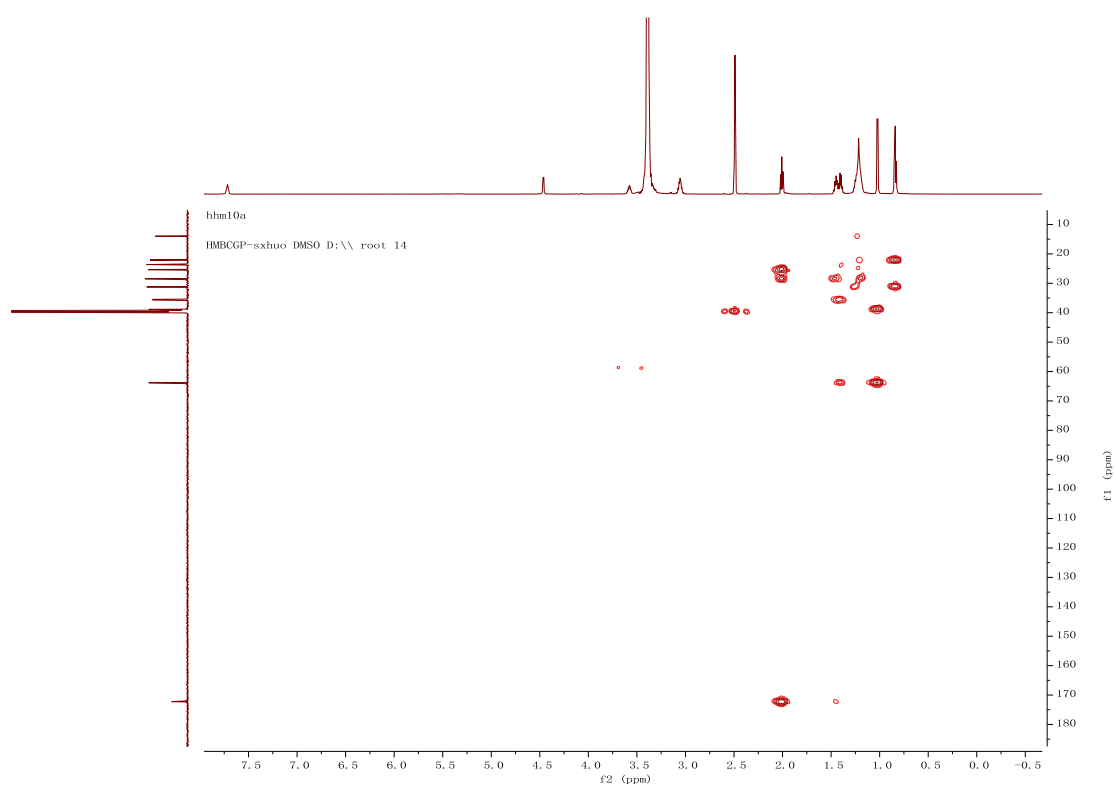


Figure S20. ^1H - ^1H COSY spectrum of compound **3** .

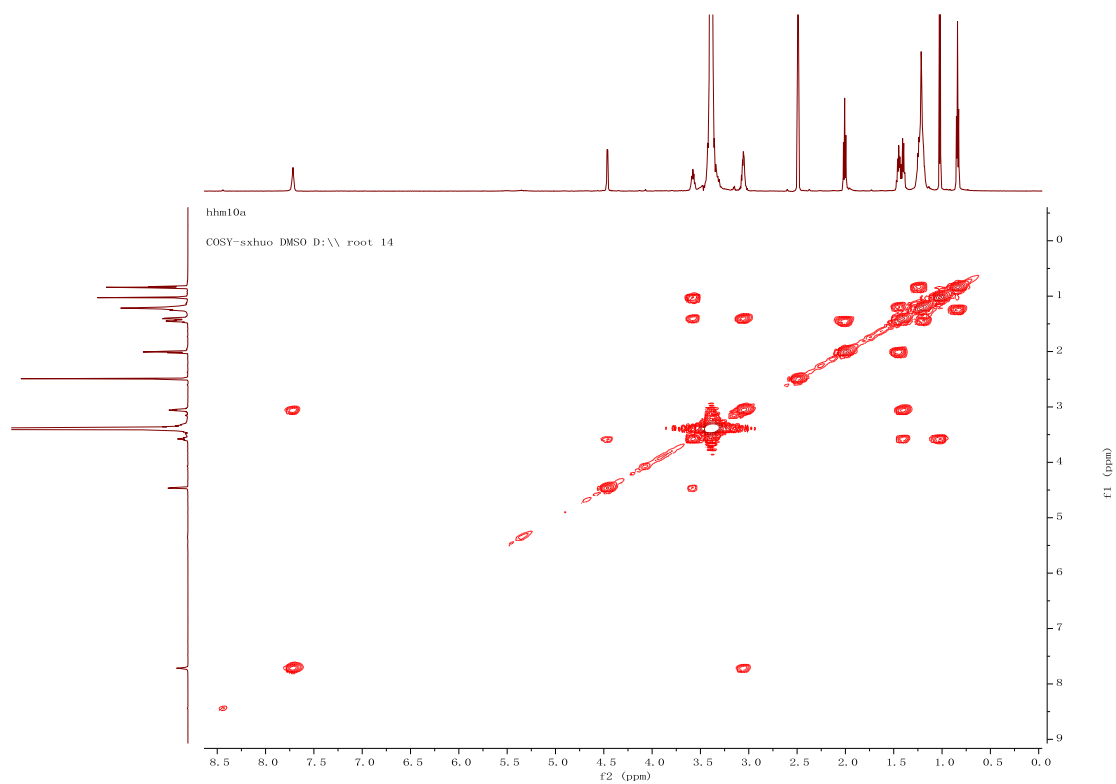


Figure S21. ^1H NMR spectrum of compound **4** ($\text{DMSO}-d_6$).

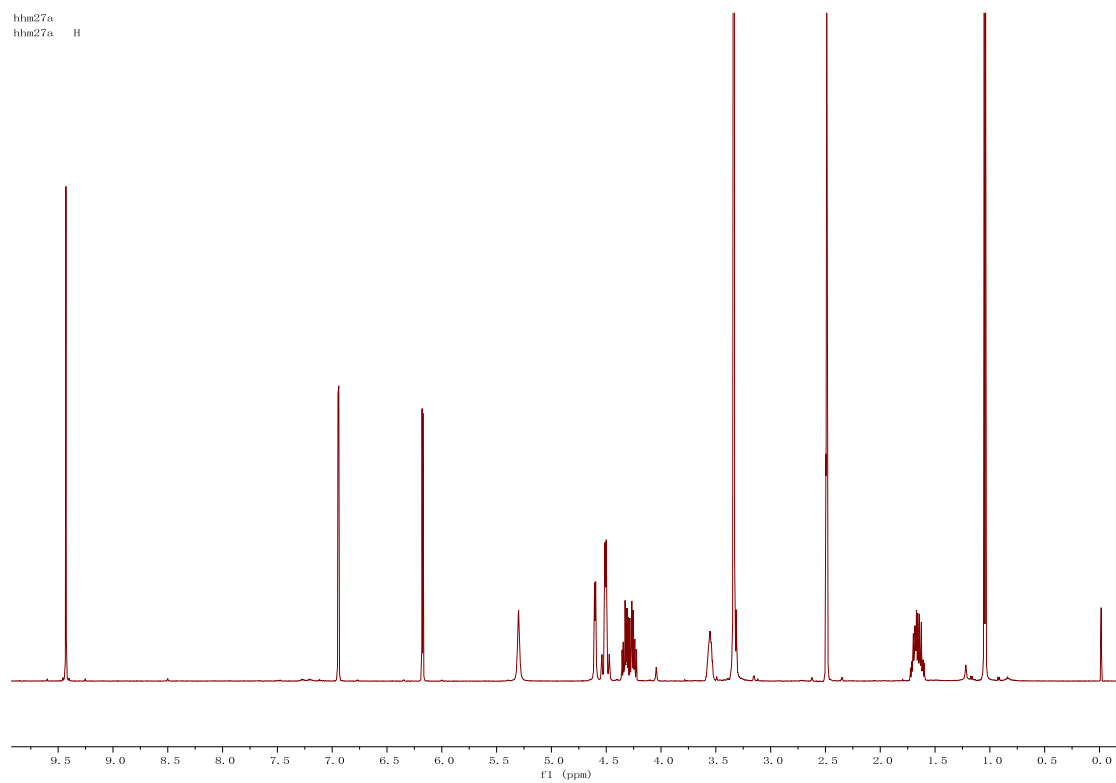


Figure S22. ^{13}C NMR and DEPT spectrum of compound **4** ($\text{DMSO}-d_6$) .

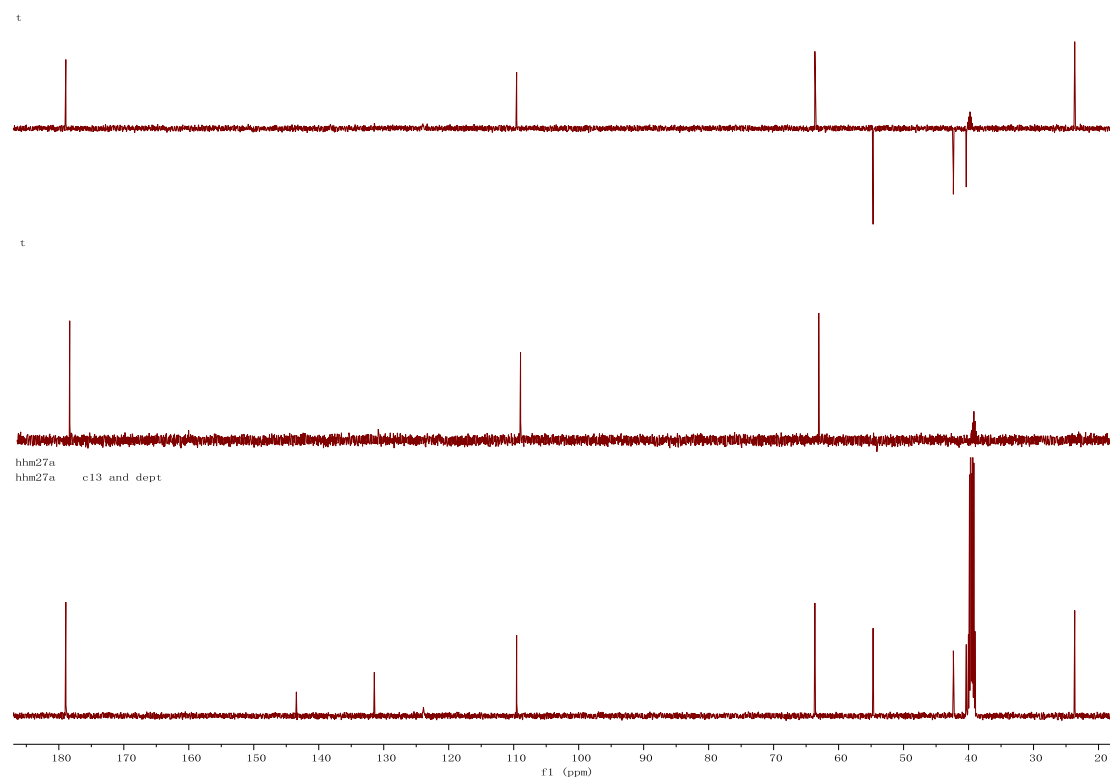


Figure S23. HSQC spectrum of compound **4** .

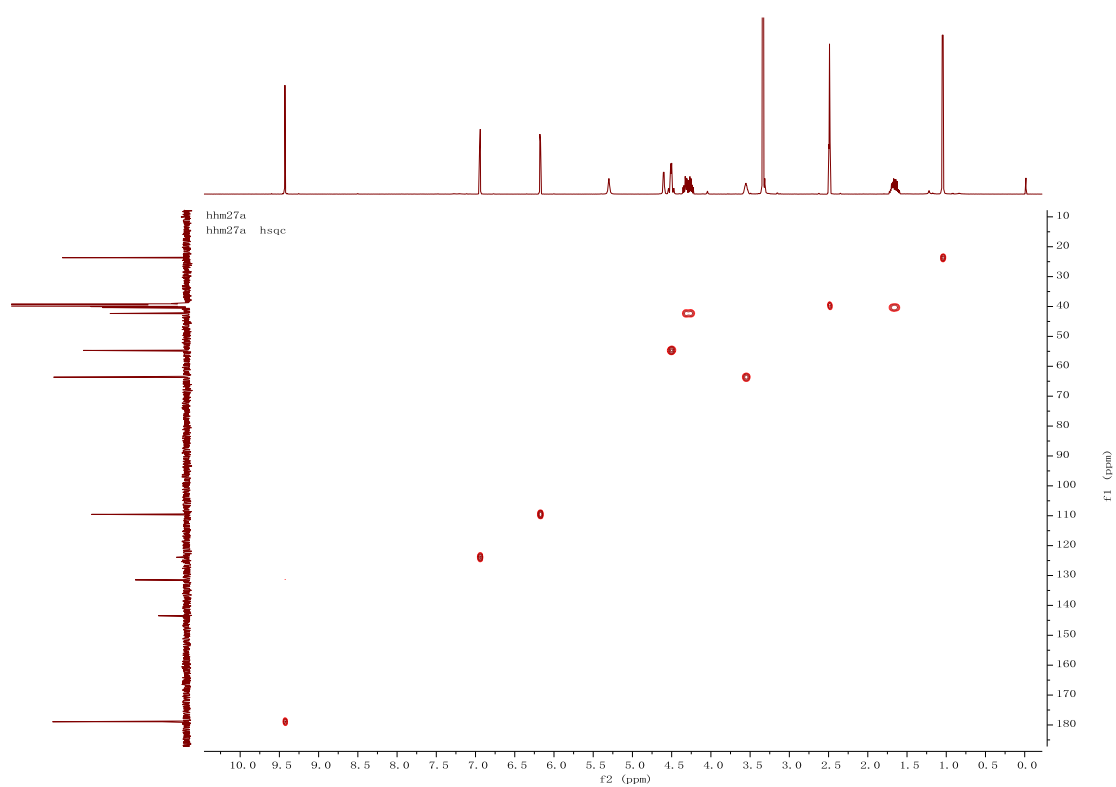


Figure S24. HMBC spectrum of compound **4** .

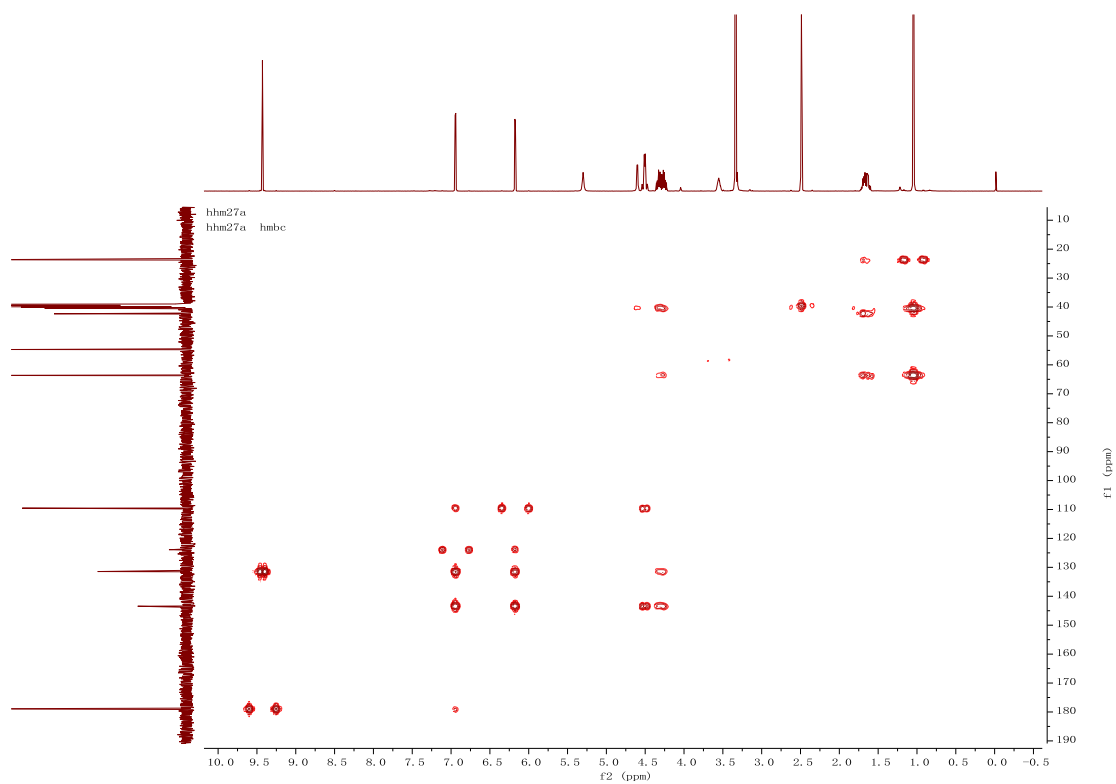


Figure S25. ^1H - ^1H COSY spectrum of compound 4 .

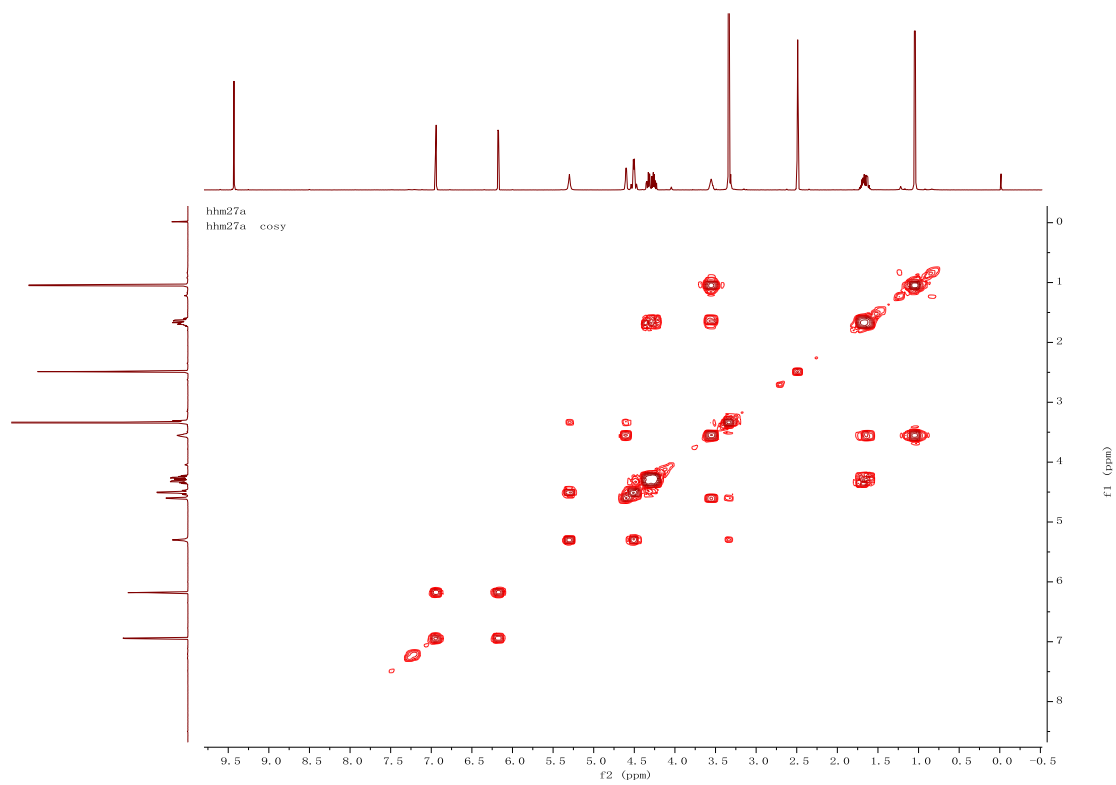


Figure S26. ^1H NMR spectrum of compound 5 (Acetone) .

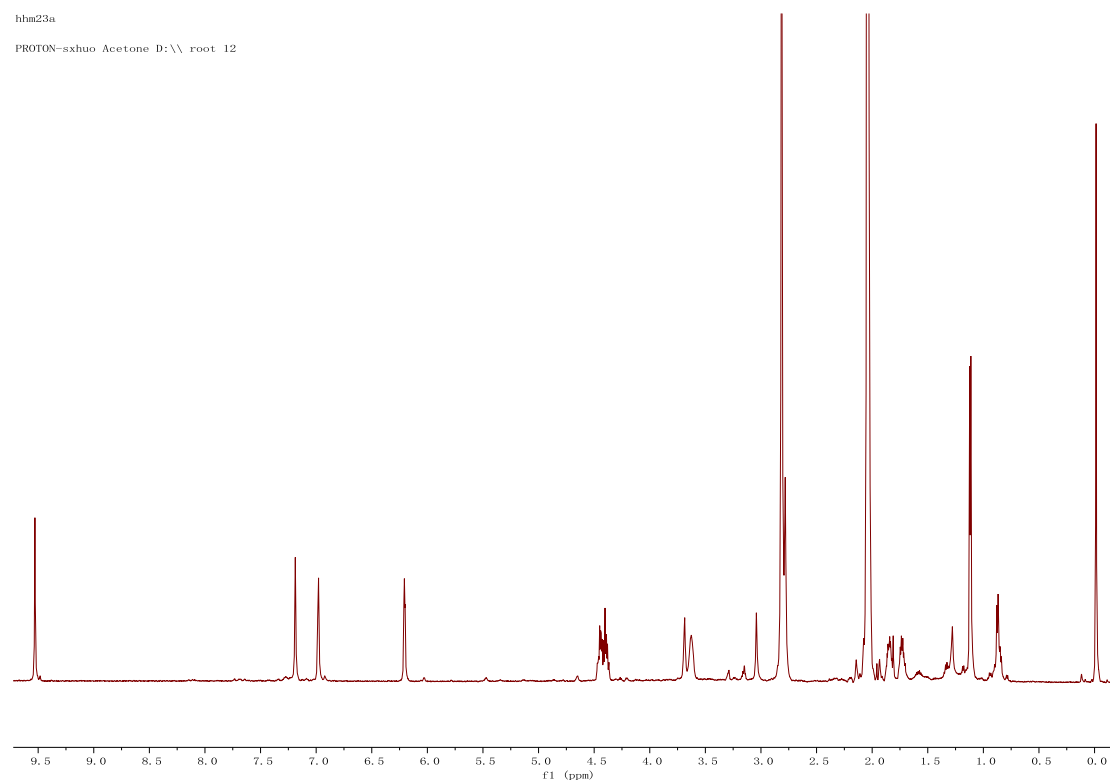


Figure S27. ^{13}C NMR and DEPT spectrum of compound 5 (Acetone) .

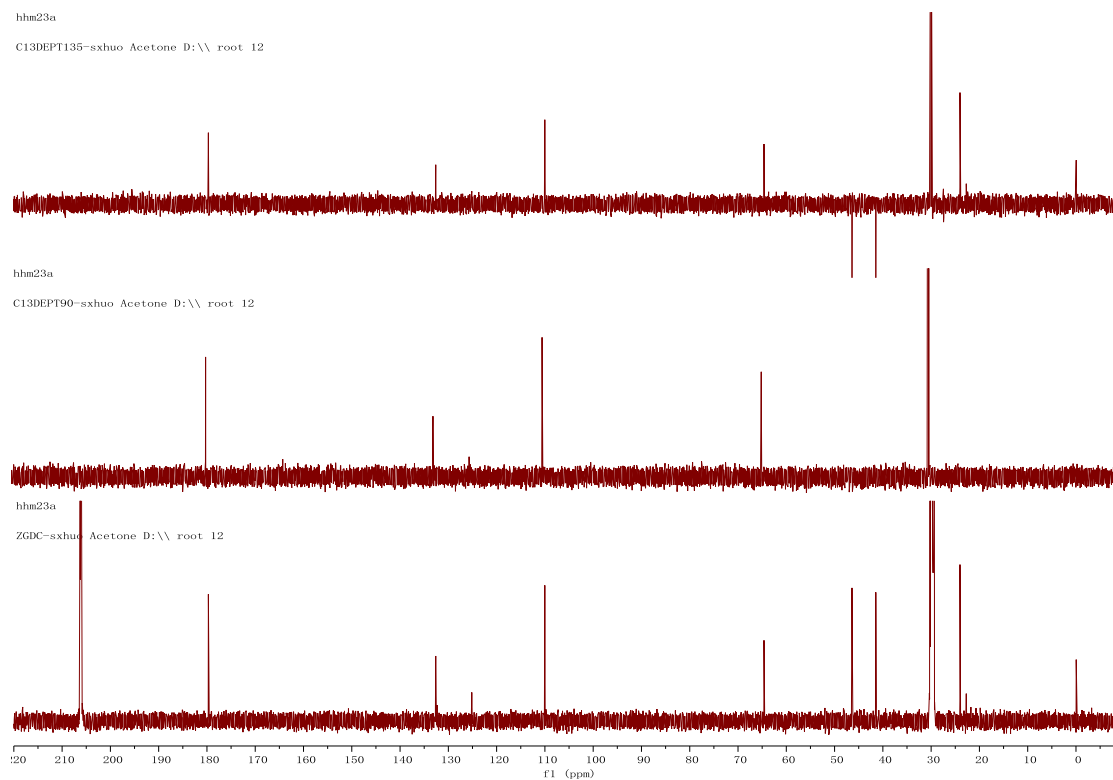


Figure S28. HSQC spectrum of compound 5 .

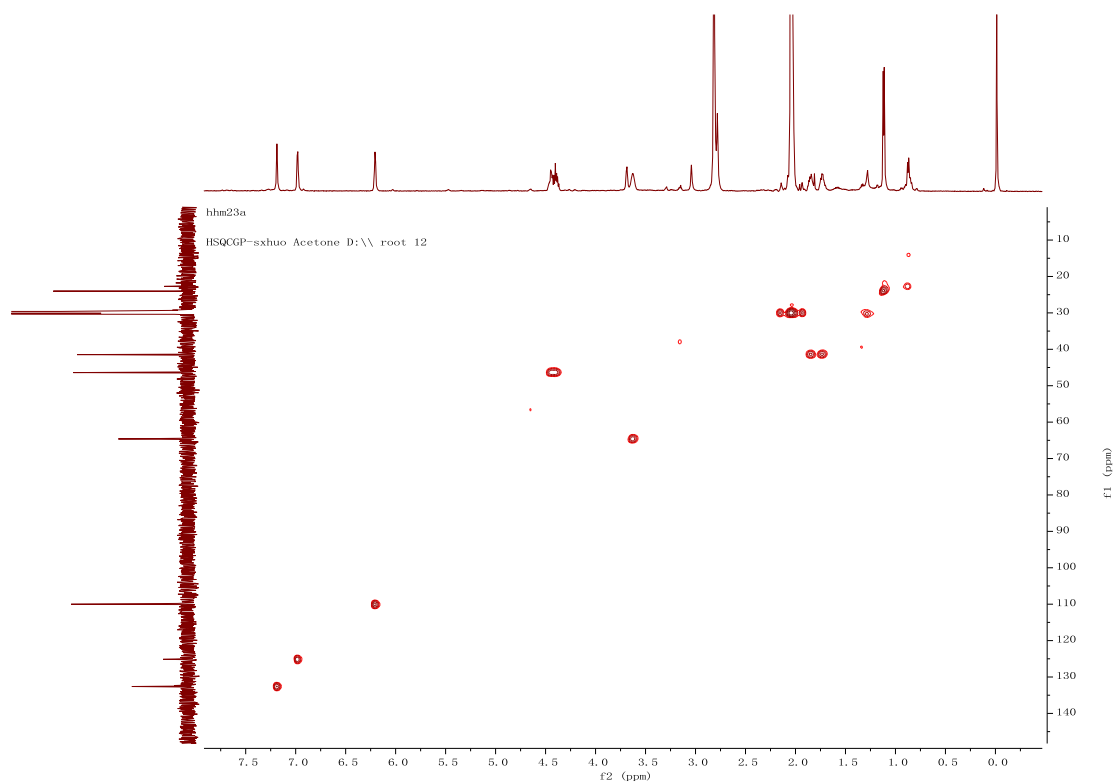


Figure S29. HMBC spectrum of compound 5 .

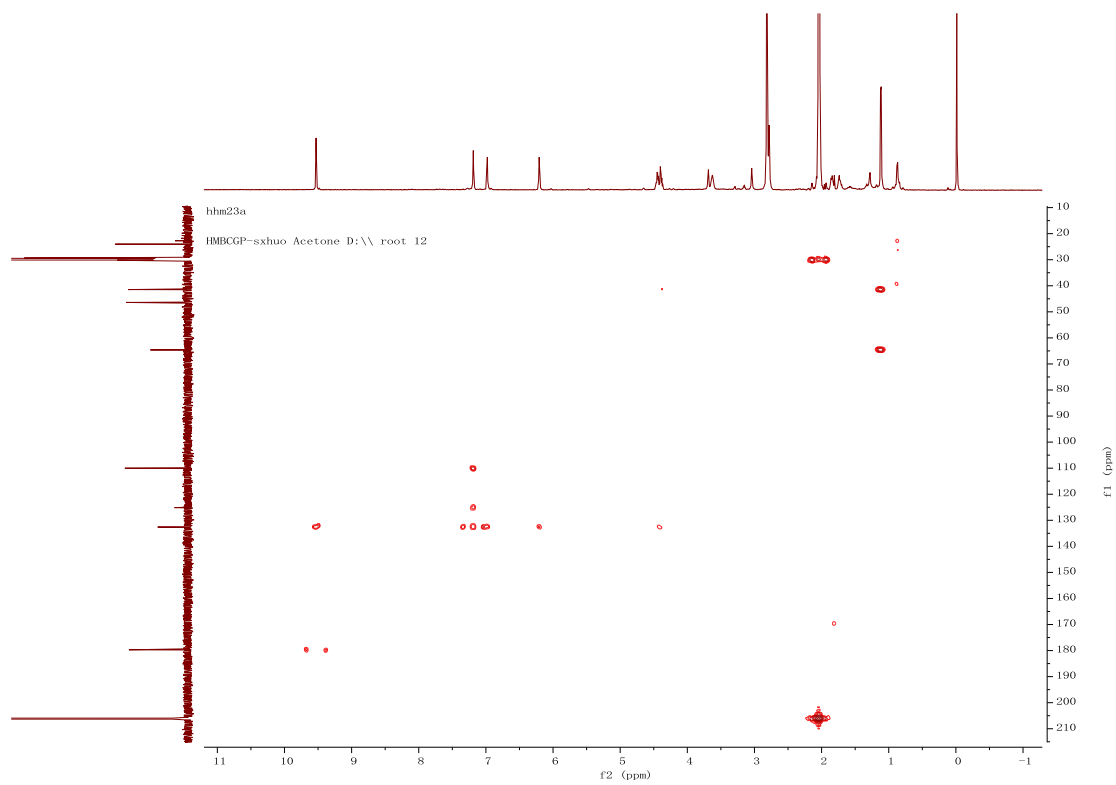


Figure S30. ^1H - ^1H COSY spectrum of compound **5** .

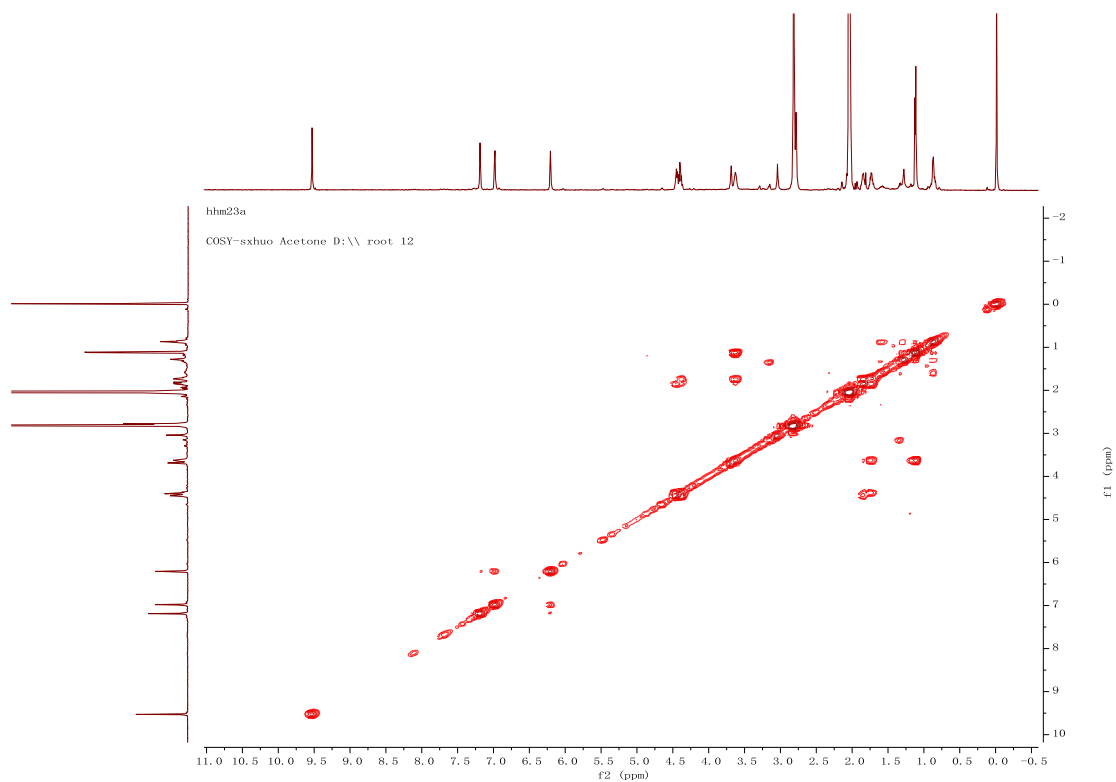


Figure S31. ^1H NMR spectrum of compound **6** (DMSO- d_6) .

hbm28a
h DMSO av600

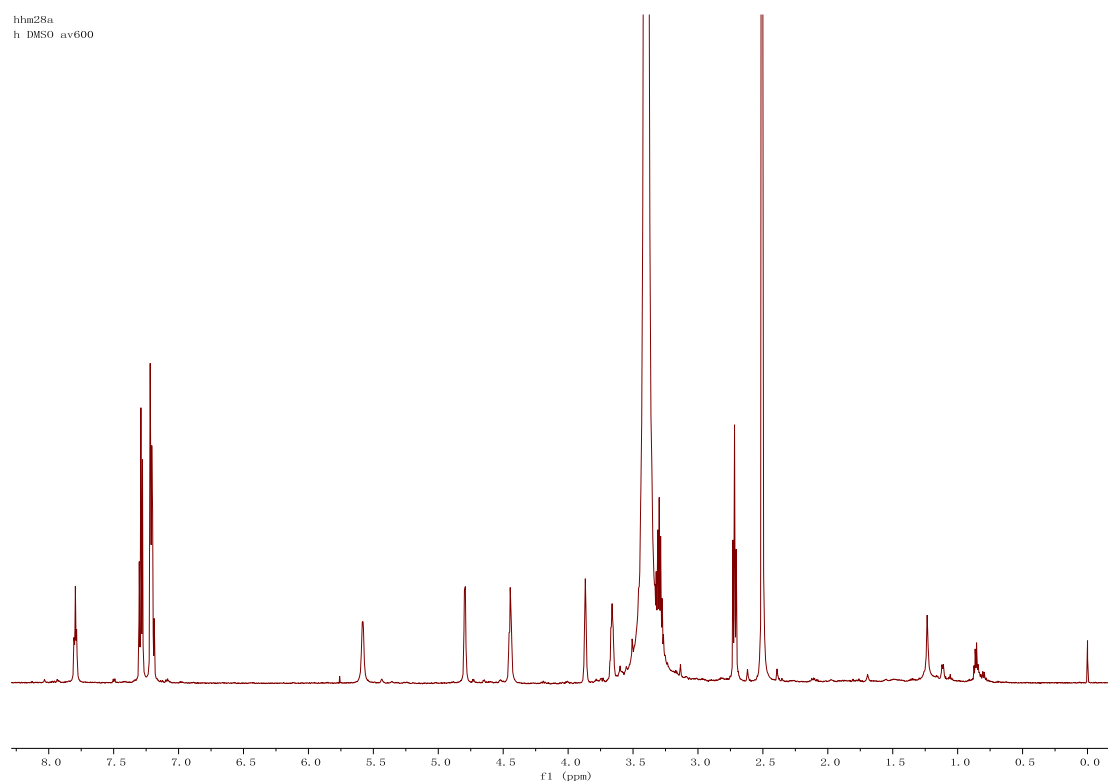


Figure S32. ^{13}C NMR and DEPT spectrum of compound 6 ($\text{DMSO-}d_6$) .

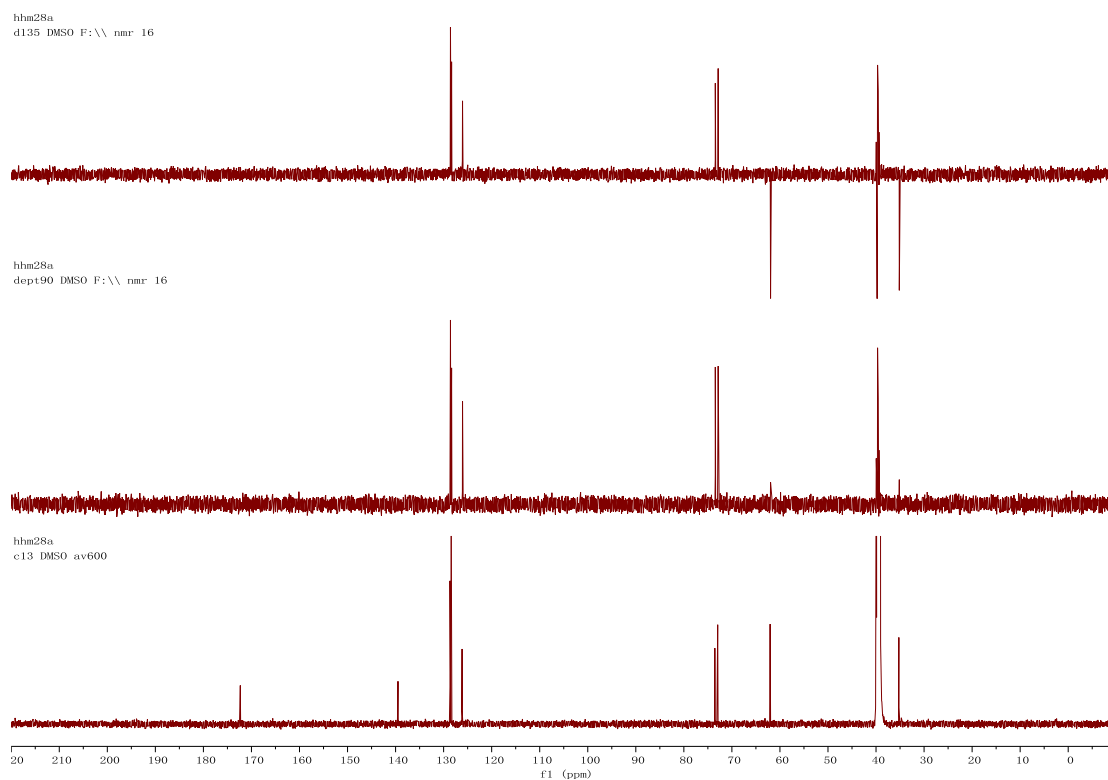


Figure S33. HSQC spectrum of compound **6** .

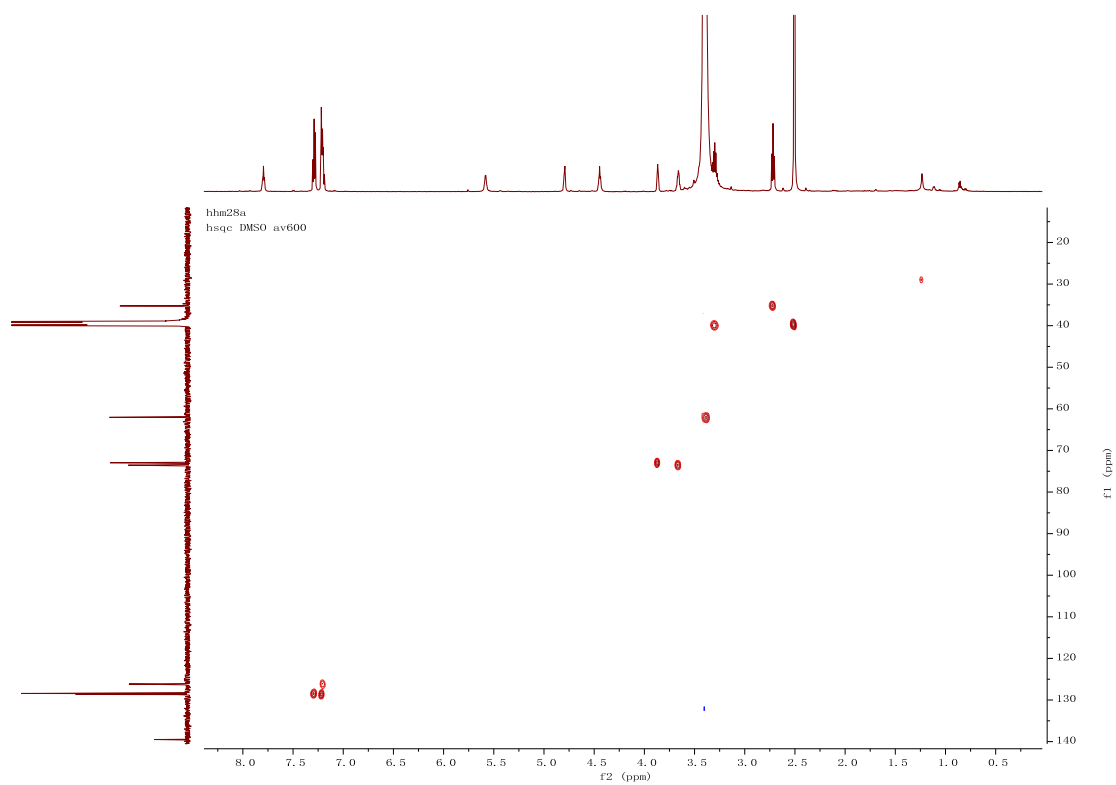


Figure S34. HMBC spectrum of compound **6** .

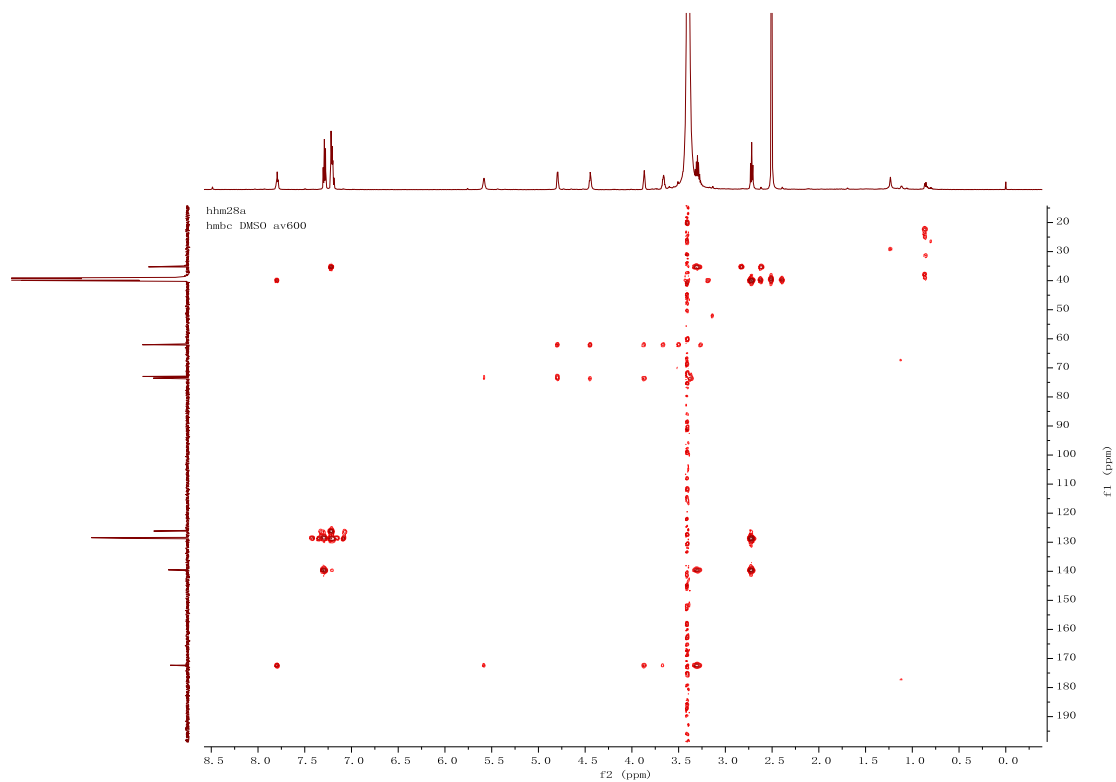


Figure S35. ^1H - ^1H COSY spectrum of compound **6** .

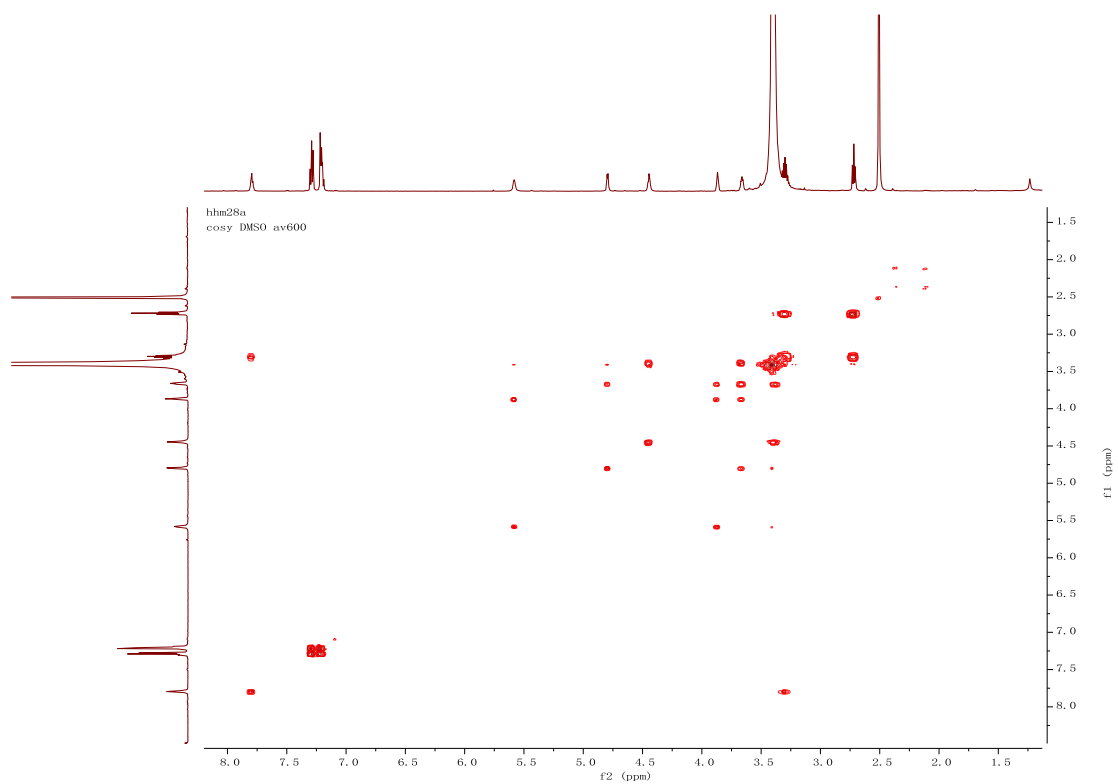


Table S1. ^1H and ^{13}C NMR Data (δ) of Compound **1** (δ in ppm and J in 800 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1	176.0	
2	34.8	2.31 (t, 7.44)
3	26.0	1.60 (m)
4	30.1	1.32 (m)
5	25.5	1.60 (m)
6	41.0	2.59 (t, 7.36)
7	203.9	
8	128.8	6.12 (d, 15.6)
9	145.3	7.23 (dd, 15.6, 9.68)
10	147.4	6.27 (ddd, 21.44, 15.2, 6.4)

11	130.3	6.27 (ddd, 21.44, 15.2, 6.4)
12	34.1	2.20 (dd, 14, 7.12)
13	29.6	1.46 (m)
14	30.0	1.32 (m)
15	23.5	1.32 (m)
16	32.6	1.32 (m)
17	14.3	0.91 (t, 6.96)
OCH ₃	52.0	3.64 (s)

Table S2. ^1H and ^{13}C NMR Data (δ) of Compound **2** (δ in ppm and J in 600 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1	171.62	
2	35.45	2.05 (t, 7.74)
3	23.27	2.19 (dd, 7.2, 14.46)
4	128.53	5.27 (m)
5	130.28	5.31 (m)
6	26.60	1.97 (dd, 6.9, 13.92)
7	28.81	1.26 (m)
8	30.92	1.23 (m)
9	22.03	1.24 (m)
10	13.99	0.84 (t, 6.84)
1'	35.77	3.06 (m)
2'	38.83	1.40 (m)
3'	63.81	3.58 (m)
4'	23.63	1.02 (d, 6.18)

Table S3. ^1H and ^{13}C NMR Data (δ) of Compound **3** (δ in ppm and J in 600 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1	172.24	
2	35.46	2.01 (t, 7.38)
3	25.37	1.45 (m)
4	28.47	1.21 (m)
5	28.64	1.21 (m)

6	31.23	1.21 (m)
7	22.10	1.23 (m)
8	14.00	0.84 (t, 6.84)
1'	35.71	3.06 (m)
2'	38.86	1.40 (m)
3'	63.82	3.57 (m)
4'	23.63	1.02 (d, 6.18)

Table S4. ^1H and ^{13}C NMR Data (δ) of Compound **4** (δ in ppm and J in 500 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1		
2	131.45	
3	123.94	6.94 (d, 3.95)
4	109.54	6.17 (d, 3.95)
5	143.44	
1'	42.33	4.29 (m)
2'	40.35	1.66 (m)
3'	63.65	3.55 (m)
4'	23.66	1.04 (d, 6.2)
1''	54.69	4.50 (dd, 13.7, 19.6)
2-CHO	178.92	9.43 (s)

Table S5. ^1H and ^{13}C NMR Data (δ) of Compound **5** (δ in ppm and J in 600 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1		
2	132.34	
3	125.14	6.98 (d, 3.9)
4	110.02	6.20 (dd, 2.34, 3.78)
5	132.61	7.19 (brs)
1'	46.40	4.42 (m)
2'	41.46	1.84 (m), 1.73 (m)
3'	64.62	3.62 (m)
4'	24.03	1.12 (d, 6.12)
2-CHO	179.71	9.53 (s)

Table S6. ^1H and ^{13}C NMR Data (δ) of Compound **6** (δ in ppm and J in 600 Hz)

Position	$\delta(\text{C})$	$\delta(\text{H})$
1	35.25	2.72 (t, 7.5)
2	39.78	3.30 (m)
3		

4	172.32	
5	72.95	3.87 (s)
6	73.54	3.67 (m)
7	62.04	3.39 (m)
1'	139.50	
2',6'	128.66	7.29 (t, 7.68)
3',5'	128.42	7.21 (m)
4'	126.16	7.21 (m)
